SOLVEX : THE SOLVENT EXTRACTION DATABASE
The Past, the Present and the Future.

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SOLVEX - The Solvent Extraction Database. The Past, the Present and the Future.

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Abstract.

SOLVEX - The Solvent Extraction Database has been established at Warren Spring Laboratory, in association with a consortium of member companies of the Mineral Industry Research Organisation (MIRO), since 1974. The project was originally initiated to fulfil the need for a comprehensive source of quantitative information, on Solvent Extraction, compiled into a standard format.

Originally the data were presented in an indexed loose leaf form. Computerisation offered considerably enhancement of both the value of the database and the facilities that could be offered. However, many commercial databases available today fail to provide a method for simple data retrieval; they rely substantially on users familarising themselves with, sometimes quite complex, query languages and the precise structure of the database. Therefore to overcome this problem the computerisation process for SOLVEX included the development of a menu-driven user interface to allow rapid, selective data retrieval and reporting.

At the start of the project the bulk of the data concentrated upon distribution and kinetic data for the base metals. Since the computerisation procedure has been completed and to support the increasing industrial interest, the range of data covered has been expanded to cover nearly all metals particularly the exotics.

The database is not restricted to performance data alone, a significant proportion of the data is concerned with the physical properties of reagents, and on physicochemical data such as viscosity, interfacial tension, solubility, specific gravity and toxicity. In addition there are comprehensive sections on commercial information and references.

The database provides a qualitative guide towards the development of Solvent Extraction processes. It can be used to eliminate unsuitable reagents and to help the process designer define the optimum experimental conditions.

This paper details the structure and development of the database. The benefits such a system offers to both the process designer and reagent manufacturer are discussed. Future plans for database development are outlined.

Introduction.

Solvent Extraction data can and are presented in a variety of formats ranging from a simple tabular layout to isothermal plots and complex triad graphs for partially miscible systems. Comparison of data from such a variety of sources can be both time consuming and laborious. Nevertheless, flowsheet design or evaluation requires a knowledge of equilibrium data for such systems. This usually demands some experimental work but a comprehensive literature search can often provide a guide to the likely optimum operating conditions and so reduce the amount of experimental work necessary.

In addition, the process designer may be faced with considerable problems regarding reagent selection. A large number of reagents are available, from a variety of manufacturers, world wide. As well as equilibrium data, the process designer must also consider factors such as the loading capacity of the extractant, its selectivity for the desired solute over any impurities which may be present, its availability, safety and, not least, its cost. The physicochemical properties of the system may be important, those with high interfacial tensions and low viscosity are always helpful to promote good phase separation. Collation and evaluation of this type of data may well involve considerable time and expense.

The Solvent Extraction Database, SOLVEX, was set-up in response to these problems, offering a single comprehensive source of reliable, quantitative information compiled into a standard format [Ref 1].

SOLVEX has been established at Warren Spring Laboratory, in association with a consortium of member companies of the Mineral Industry Research Organisation (MIRO), since 1974. Its longevity reflects the success of the service. The database consists of a huge reference library of kinetic and distribution data. A considerable proportion of the database is concerned also with physical properties of reagents and physicochemical data such as specific gravity, interfacial tension, viscosity, solubility and toxicity. There are also comprehensive sections on commercial information and references.

As well as being beneficial to the process designer, SOLVEX, has much to offer the reagent manufacturer. Its configuration and design can be used to investigate the relationships between reagent structure and function and so assist in the development of new reagents. It can also help to identify gaps in the market where new reagents could be welcomed by the solvent extraction industry.

History.

In 1974 SOLVEX was established as a database for solvent extraction information. The project is managed as an industrial club project with access being restricted to club members.

Orginally the database was presented in a series of indexed loose leaf folders so that amending and updating could be achieved relatively easily. It was recognised from the start of the project that the value of the system could be greatly enhanced if the system could be transfered to a computer for storage and access. However, at that time both hardware and software were highly expensive and the benefits to be gained did not justify the cost. Within ten years the amount of data collected had become unmanageable and the cost of introducing computerisation had dropped considerably. By the end of 1984 club members had taken the decision to transfer the database to a computerised Relational Database Management System. The database was to be stored on the laboratory's central mini computer, a GEC 63/30 and would be built using the Empress/32 system utilising the fourth generation language 'Mbuilder' and interfacing with both Fortran and C computer languages.

Computerisation, together with the development of a unique menu-driven user interface to allow rapid and selective 'user-friendly' data retrieval was completed in 1987. The full remote system was then available to club members via a data communication system, either Packet Switch Stream (PSS) or Public Switched Telephone Network (PSTN).

Any database is only as good as the data it contains. In the early days of the project, the data within SOLVEX were mainly concerned with base metals. A few years later data for the precious metals were added. All information was and still is updated on an annual basis from literature searches and also from Warren Spring Laboratory's own unpublished research. In addition, where gaps in data were seen, club members commissioned the laboratory to carry out experimental work to close these gaps. The results from two such projects have subsequently been published [Ref 2,3]. After computerisation the next priority was to expand the scope of the data. Currently nearly all metals are included within SOLVEX

excluding the transuranics but including gallium, germanium, indium and the rare earths. In addition the database includes data for the mineral acids as solutes.

The Structure of the Database.

A Relational Database Management System (RDBMS) is a computer program that can be used to store, organise, manipulate and retrieve large amounts of related data. Data is stored in a series of tables having a row and column format. The tables themselves can be related to one and other via cross referencing. This allows multiple tables to be accessed simultaneously.

SOLVEX currently has sixteen data tables which can be divided into three main subject areas, all of which are interrelated.

The largest area is that devoted to performance data. These tables contain distribution and kinetic data for specific solvent extraction systems. Data include a full description of all components of the solvent, solute concentrations for both phases - initially and after equilibrium, acid concentrations, pH values, temperature, phase ratio, contact time etc. In addition Distribution coefficients (D values), Log D and separation factors are calculated. Each solvent extraction system is identified by a 'Head Number'. Within the bounds of each head number several sub-sets of data, identified by 'Row Numbers', may be present. Each row number may contain data for an individiual shake out test, perhaps each test carried out at a different pH or with a different contact time.

The Extraction data table is cross referenced with another table containing references via a unique number which refers to the data source. This Reference table contains an entry for each paper, report, patent or information sheet from which data is abstracted for SOLVEX. By cross referencing with a reagent name the Suppliers table may be accessed to retrieve commercial information. This table contains contact names, addresses, telephone and telex numbers of companies marketing the reagents.

The second largest area within SOLVEX is that containing physicochemical data. There are nine tables storing data for interfacial tension, specific gravity, solubility, toxicity, and viscosity. This area is also linked to both the Reference table and the Suppliers table.

The third area contains physical information on reagents i.e. extractants, diluents and modifiers. Data such as molecular weights, structures, flash points, boiling points,

pour points and additives are stored. This data area is linked to both the previous two via reagent names. Again there are cross references to the Reference and Supplier tables. Figure 1 shows the structure of the database diagramatically.

Data Collection.

Suitable information for SOLVEX is continuously being collated via literature searches and Warren Spring Laboratory's own research programmes. Abstraction is carried out using an electronic graph pad and mouse interfaced to calculation software. This introduces the minimum amount of error to the data and is considerably quicker than manual techniques. The data entry package for SOLVEX includes error checking and a simple mass balance to ensure data are as accurate as possible. However, the data can only ever be as accurate as the original published material.

The loose leaf indexed database of the early SOLVEX days has been maintained and all club members are issued with new and updated data, as hardcopy, on a regular basis.

Table 1 shows the current data content of SOLVEX. Figure 2 illustrates the breakdown of the Extraction table in terms of solutes.

Table 1 : The data content of SOLVEX

Data Area	Approx. No. Records
Extraction	40,000
Physico-chemical	2,000
Reagent	300
Reference	1000
Supplier	50
Database management	5,000
Application building	7,000
Interface programmes (75) =	55,000

Data Retrieval.

Traditionally a database management system has an associated structured query language (SQL) which allows the data tables to be interrogated. These query languages are usually rich, powerful and flexible but in order to utilise them sucessfully the user requires a detailed knowledge of the language, the database structure and a basic understanding of computer operation. Different databases may well require a knowledge of a different SQL. Subsequently database interrogation is often left to specialised personnel such as library staff or computer operators. Many a commercial database has fallen into this trap and often much of the intended benefits, such as speed and information 'on tap' are lost.

SOLVEX overcomes this problem by offering an alternative method of inquiry via a unique menu-driven retrieval system. This system has been designed and implemented using a fourth generation computer language (4GL), Mbuilder. Mbuilder offers a windowing and menu utility which is fully integrated into SOLVEX via the FORTRAN and C computer languages. consequently, this system offers SOLVEX users a rapid, selective data retrieval and reporting facility without the need for any knowledge of a computer language or the database structure.

This is not to say that the EMPRESS/32 query language is obsolete. The menu-driven system can only cover the more routine queries and can only be used in run-time mode. For custom built queries, those running in batch mode or for time consuming queries commissioned to run during the computer's 'quiet hours' the query language is used.

Another problem commonly associated with commercial databases is the search mechanism. Often complex queries are initially presented which take considerable time to process and may well fail due to either lack of data or to the format of the query. SOLVEX breaks each query down into a series of stages, each stage can be processed rapidly and in the case of failure at an early stage alternative, similar data are offered to the user. This technique prevents unnecessary and expensive computer connect time.

To use the menu driven retrieval system, the user selects options from a series of menus and types the answers to simple questions such as those requesting the user to enter the extractant name or the chemical formula of the solute. Figure 3 shows a flowchart of a simple query and how SOLVEX retrieves data. Error checks are continuously performed on the user input and redundant keyboard keys are immobilised to prevent accidental computer crashes. A comprehensive help text is available at all search levels and access to the database

manager is available via the electronic mail facility SOLVEX offers its users.

Hardware and Access to SOLVEX.

The choice of computer hardware must always be the responsibility of the end user, Warren Spring Laboratory can only take an advisory role. The recommended terminal to use with SOLVEX is either a DEC VT preferably from the 200 or 300 series or one of the Tektronics 4200 series. Often users prefer to use a PC as a terminal, in this case emulation software will be necessary. Providing the emulator is configured correctly there are few problems with this approach. In addition, most users will require a printer compatible with their chosen terminal to allow screen dumps of their retrieved data.

SOLVEX is accessed via the laboratory's data communication network - OSNET. This is an Ethernet Local Area Network from ICL implementing the latest standards as defined by the International Standards Organisation. There are two methods of accessing the network and SOLVEX, either PSS or PSTN (or the international versions IPSS and IPSTN). Both are readily available from telephone authorities.

PSS is a modern system designed to handle transfer of high speed data between computers. It is, in practice, the cheapest and the least prone to errors caused by electronic noise. PSTN allows access to remote computers via a modem and telephone. This technique converts computer output signals to and from audio tones which can then be sent over normal telephone lines. Unfortunately this is prone to noise errors and is only suitable for slow speed communication. Therefore, it is not recommended for SOLVEX users overseas.

Future plans for the database include development of a graphical interface. When this is available users will require a colour graphics terminal or colour graphics card for their PC in order to receive the full facility.

Data and Computer Security.

Access to the WSL network requires the knowledge of the network user address number (NUA) and a unique authorisation identity code (AIC). Each SOLVEX customer has a unique 'Login name' and password. These are all issued to members on joining the SOLVEX club. The user password is changed on a regular basis. Access to the data within the database can only be achieved by entering a further password which is again

changed regularly.

The Empress system utilises a comprehensive security mechanism by which the database manager can grant or deny certain privileges to users. SOLVEX members may only read data, they may not add, amend or delete data. Only the database manager has these privileges.

Future Plans.

Over recent years SOLVEX has grown both in membership terms and in terms of the huge amount of data stored. The full cost of the service is born by club members and so the larger the membership the lower the subscription cost. Due to recent increases in subscribers, SOLVEX members are currently able to considering enhancing the facilities of the system without dramatically increasing the annual cost. It is proposed to develop a graphics interface which is fully integrated into the present system. This would greatly enhance the visual impact of the database and allow easier comparisons of performance data and bring SOLVEX to the forefront of database technology.

In addition to this development phase, annual data updates and the production of hardcopies will continue, as will the usual care, maintenance and project management. At regular intervals a newsletter will be issued to keep club members and other interested parties informed of both SOLVEX and other solvent extraction news.

Conclusion.

The longevity of the SOLVEX project has shown that industry has a need for a single comprehensive source of reliable quantitative information on solvent extraction, compiled into a standard format. SOLVEX satisfies these requirements and sucessfully overcomes many of the problems associated with other commercial databases. The database is targeted specifically at the solvent extraction industry and is of benefit to flowsheet designers, evaluators and manufacturers alike.

References.

1. Collins, D.N., Flett, D.S., Melling, J. and Barber, S.P.
    1986, Reagent Databases for the Metallurgical Industry.
    Proceedings of a Symposium: Advances in Mineral Processing,
    New Orleans, USA. Chapter 22, Pages 380-394

2. Flett, D.S. and Melling, J.
    1979, Extraction of ammonia by commercial copper chelating
    extractants.   Hydrometallurgy, Volume 4, Pages 135-146

3. Flett, D.S., Melling, J. and Itoh, E.
    1983, Solvent extraction of cobalt and nickel by a phosphonic
    acid ester.   International Solvent Extraction Conference,
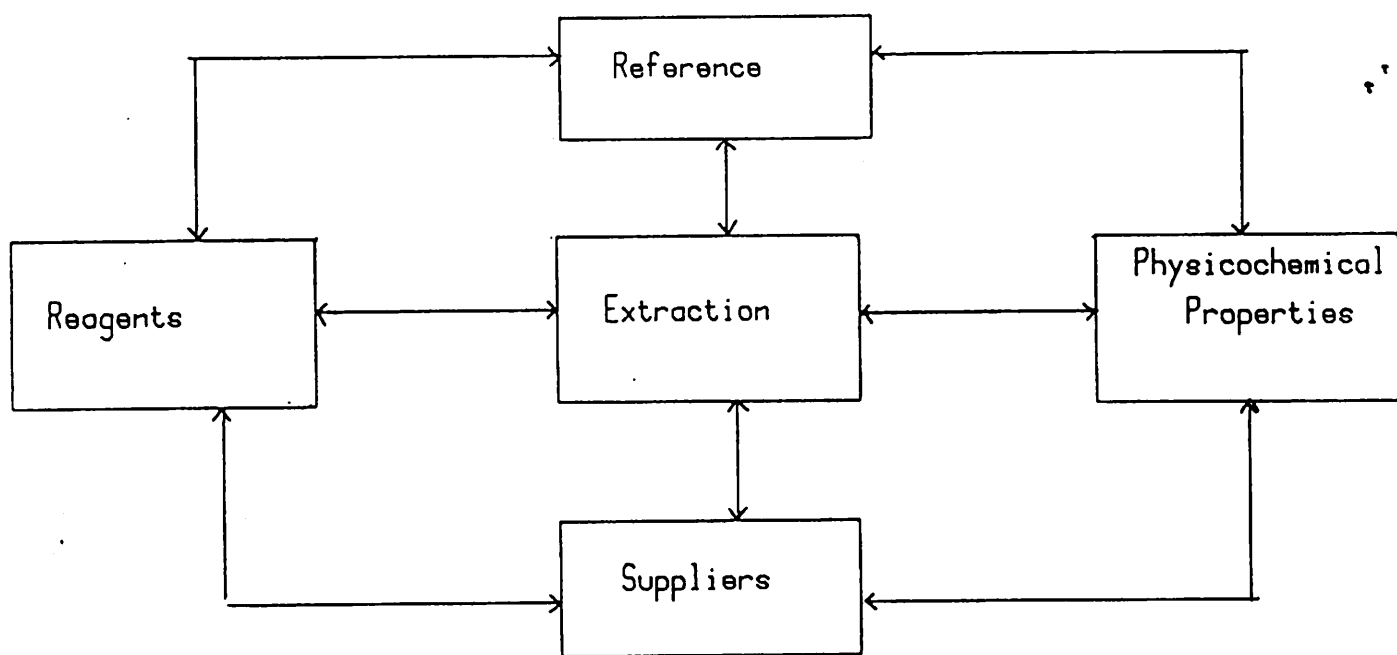   ISEC '83, proceedings, AIChE,   Pages 232-233
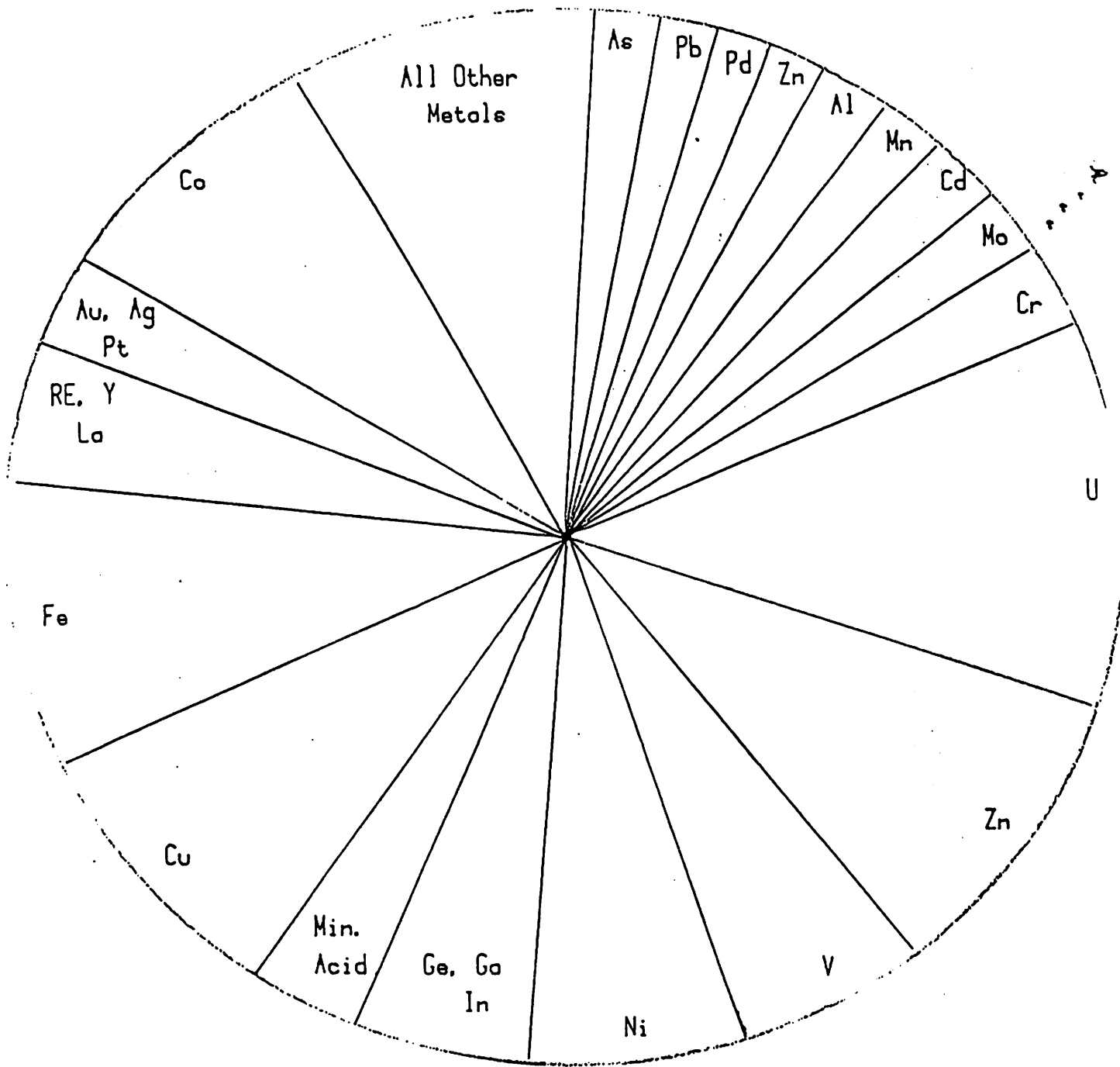
Figure 1: The Structure of SOLVEX
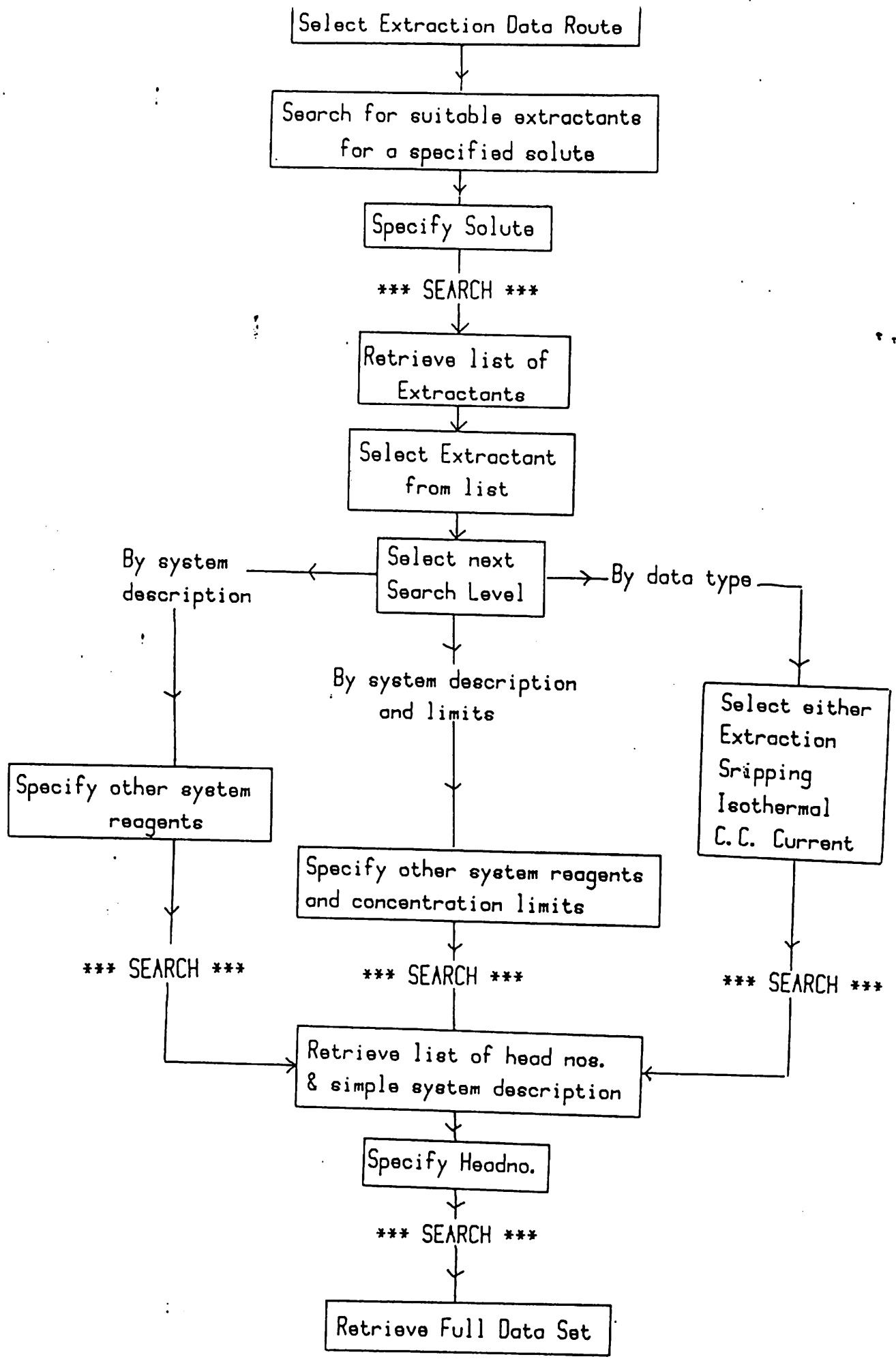
Figure 2: Distribution of Solutes in the Extraction table

Figure 3 : Flowchart of a Simple Query.